MATHEMATICAL METHODS OF QUANTUM MECHANICS SUMMARY

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Abstract.

Contents

Postulates of Quantum Mechanics

Quantum mechanical system	separable Hilbert space $\mathscr{H}$
State	$\psi \in \mathscr{H}, \lVert\psi\rVert = 1$
Observables	Self-adjoint operators on $\mathscr{H}$
Expected Value of an observable A in the state ψ	$\langle\psi, A\psi\rangle$
Variance of an observable A in the state ψ	$\Delta A_\psi := \langle\psi, A^2\psi\rangle - \langle\psi, A\psi\rangle^2$

Lemma 1.1 (Heisenberg Uncertainity Principle). *Let A and B two self-adjoint operators on a Hilbert space $\mathscr{H}$. Then for any state ψ*

$$\Delta A_\psi \Delta B_\psi \geq \frac{1}{4} |\langle\psi, [A, B]\psi\rangle|^2 .$$

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Unbounded Operators

Definition 1.1 (Linear Operator). *Let $\mathscr{H}$ be a Hilbert space. A **(linear) operator on $\mathscr{H}$** is simply a linear map $A : D(A) \to \mathscr{H}$, where $D(A)$ is a linear subspace of $\mathscr{H}$.*

Examples 1.1.

(a) (***Multiplication operator***) Let $\mathscr{H} := L^2(\mathbb{R})$ and consider $\widehat{x} : D(\widehat{x}) \to L^2(\mathbb{R})$ defined by $(\widehat{x}\psi)(x) := x\psi(x)$ (or $(\widehat{f}\psi)(x) := f(x)\psi(x)$ for any complex valued measurable function f).

(b) (***Differential operator***) Let $\mathscr{H} := L^2(\mathbb{R})$ and consider $\nabla : C^\infty(\mathbb{R}) \to L^2(\mathbb{R})$.

Definition 1.2 (Closed Operator). *An operator A on $\mathscr{H}$ is said to be **closed**, iff Γ_A is closed in $\mathscr{H} \times \mathscr{H}$.*

Definition 1.3 (Closable Operator). *An operator A on $\mathscr{H}$ is said to be **closable**, iff $\overline{\Gamma}_A$ is a linear graph, i.e. $(0, y) \in \overline{\Gamma}_A$ implies $y = 0$. The corresponding operator associated to $\overline{\Gamma}_A$ is denoted by $\overline{A}$ and called the **closure** of A. Clearly $A \subseteq \overline{A}$.*

Definition 1.4 (Adjoint). *Let A be a densly defined operator on $\mathscr{H}$. Set*

$$D(A^*) := \{\psi \in \mathscr{H} : \exists \eta \in \mathscr{H} \text{ s.t. } \forall \varphi \in D(A)\ \langle A\varphi, \psi\rangle = \langle \varphi, \eta\rangle\},$$

*and $A^*\psi := \eta$. The operator A^* is called the **adjoint** of A.*

Theorem 1.1. *Let A be a densly defined operator on $\mathscr{H}$. Then:*

(a) A^* is closed.

(b) A is closable if and only if $D(A^*)$ is dense.

(c) If A is closable, then $(\overline{A})^* = A^*$.

Definition 1.5 (Symmetric Operator). *A densly defined operator A is said to be **symmetric**, iff $A \subseteq A^*$.*

Definition 1.6 (Self-adjoint Operator). *A densly defined operator is said to be **self-adjoint**, iff $A = A^*$.*

Example 1.1. Let A_f denote the multiplication operator. Then $A_f^* = A_{\bar{f}}$.

Definition 1.7 (Essentially Self-adjoint Operator). *A symmetric operator A is said to be **essentially self-adjoint**, iff $\overline{A}$ is self-adjoint.*

Example 1.2. Let $\mathscr{H} := L^2[0, 2\pi]$ and consider the operator A defined by $A := -i\frac{d}{dx}$ with $D(A) := \{\psi \in C^1[0, 2\pi] : \psi(0) = \psi(2\pi)\}$.

Theorem 1.2. *Let A be a symmetric operator. Then the following statements are equivalent:*

(a) A is self-adjoint.

(b) A is closed and $\ker(A^* \pm i) = \{0\}$.

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(*c*) $\operatorname{im}(A \pm i) = \mathcal{H}$.

There is a way of defining uniquely self-adjoint extensions of symmetric non-negative operators (***Friedrichs extension***).

Lemma 1.2 (Weyl Lemma). *Let A be a closed densly defined operator such that there exists a sequence $(\psi_n)_{n\in\omega}$ in $D(A)$ with $\|\psi_n\| = 1$ for all $n \in \omega$ and $\|(A - z)\psi_n\| \to 0$ for some $z \in \mathbb{C}$. Then $z \in \sigma(A)$ (the sequence $(\psi_n)_{n\in\omega}$ is called a **Weyl sequence**).*

Theorem 1.3. *Let A be a symmetric closed operator. Then A is self-adjoint if and only if $\sigma(A) \subseteq \mathbb{R}$.*

The Spectral Theorem

Definition 1.8 (Projection Valued Measure). *Let $\mathcal{H}$ be a Hilbert space. A function*

$$P : \mathcal{B}(\mathbb{R}) \to \mathcal{L}(\mathcal{H})$$

*is said to be a **projection valued measure**, iff*

(*i*) *For all $\Omega \in \mathcal{B}(\mathbb{R})$, $P(\Omega)$ is an orthogonal projection, i.e. $P(\Omega)^2 = P(\Omega) = P(\Omega)^*$.*
(*ii*) *$P(\mathbb{R}) = \mathrm{id}_{\mathcal{H}}$.*
(*iii*) *If $(\Omega_n)_{n\in\omega}$ is a sequence of pairwise disjoint elements of $\mathcal{B}(\mathbb{R})$, then*

$$P(\Omega)\psi = \sum_{n\in\omega} P(\Omega_n)\psi,$$

for all $\psi \in \mathcal{H}$.

Definition 1.9 (Resolution of the Identity). *Let $\mathcal{H}$ be a Hilbert space and P a projection valued measure. The function $p : \mathbb{R} \to \mathcal{L}(\mathcal{H})$ defined by*

$$p(\lambda) := P\,(-\infty, \lambda]\,,$$

*is called the **resolution of the identity associated to a projection valued measure**.*

Functional Calculus. Let $P : \mathcal{B}(\mathbb{R}) \to \mathcal{L}(\mathcal{H})$ be a projection valued measure. Then for any simple function $f := \sum_{k=1}^n \alpha_k \chi_{\Omega_k}$ we define

$$P(f) := \int_{\mathbb{R}} f(\lambda)dp(\lambda) := \sum_{k=1}^n \alpha_k P(\Omega_k).$$

Since the simple functions are dense in the space of *bounded Borel functions* (with respect to $\|\cdot\|_\infty$) $\mathcal{M}_b$, we can extend above definition to $\mathcal{M}_b$. Actually, this defines a C^*-algebra homomorphism.
Consider now f just a Borel function. Then we get an operator $P(f) : D(P(f)) \to \mathcal{H}$ where

$$D(P(f)) := \{\psi \in \mathcal{H} : f \in L^2(\mathbb{R}, d\mu_\psi)\}\,,$$

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defined by

$$P(f)\psi := \lim_{n\to\infty} P(f_n)\psi,$$

where $f_n := f\chi_{|f|\leq n}$. We write

$$P(f) = \int_{\mathbb{R}} f(\lambda)dp(\lambda).$$

Existence. Existence is guaranteed by *Herglotz* or *Nevanlinna* functions.

Theorem 1.4 (Spectral Theorem). *Let A be a self-adjoint operator. Then there exists a unique projection valued measure P^A such that $D(A) = \{\psi \in \mathcal{H} : \int |\lambda|^2 \, d\mu_\psi^A(\lambda) < \infty\}$ and*

$$A = \int \lambda dp^A(\lambda).$$

Theorem 1.5. *Let A be a self-adjoint operator with projection valued measure P^A. Then*

$$\sigma(A) = \{\lambda \in \mathbb{R} : \forall\varepsilon > 0 \; P^A(\lambda - \varepsilon, \lambda + \varepsilon) \neq 0)\}.$$

Definition 1.10 (Spectral Basis). *Let A be a self-adjoint operator. A family $(\psi_\iota)_{\iota\in I}$ in $\mathcal{H}$ is said to be a* ***spectral basis*** *of $\mathcal{H}$, iff $\mathcal{H}_{\psi_i} \perp \mathcal{H}_{\psi_j}$ for all $i \neq j$, where*

$$H_{\psi_i} := \{f(A)\psi_i \in \mathcal{H} : f \in L^2(\mathbb{R}, d\mu_{\psi_i})\},$$

and $\mathcal{H} = \bigoplus_{\iota\in I} \mathcal{H}_{\psi_\iota}$.

Now for any self-adjoint operator there exists a at most countable spectral basis $(\psi_\iota)_{\iota\in I}$ and a unitary operator $U : \mathcal{H} \to \bigoplus_{\iota\in I} L^2(\mathbb{R}, d\mu_{\psi_\iota})$ such that $Uf(A)U^* = f$, where f acts as a multiplication operator on each coordinate. Thus *any self-adjoint operator is unitarily equivalent to a multiplication operator*.
Moreover, for any Borel measure μ we have a decomposition

$$L^2(\mathbb{R}, d\mu) = L^2(\mathbb{R}, d\mu_{\mathrm{ac}}) \oplus L^2(\mathbb{R}, d\mu_{\mathrm{pp}}) \oplus L^2(\mathbb{R}, d\mu_{\mathrm{sc}}).$$

Quantum Dynamics

The Schrödinger Equation.

$$i\frac{d\psi}{dt} = H\psi \qquad \textbf{(Time-dependent Schödinger equation)},$$
$$H\psi = E\psi \qquad \textbf{(Stationary Schödinger equation)}.$$

Theorem 1.6. *Let $\mathcal{H}$ be a Hilbert space and $H : D(H) \to \mathcal{H}$ be self adjoint. Moreover, set $U(t) := \exp(-iHt)$ for $t \in \mathbb{R}$. Then:*

(a) $U(t)$ is a strongly continuous one parameter unitary group.

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(*b*) *The limit*

$$\lim_{t\to 0}\frac{U(t)-1}{t}\psi$$

exists if and only if $\psi \in D(H)$. *Then*

$$\lim_{t\to 0}\frac{U(t)-1}{t}\psi = -iH\psi.$$

(*c*) $U(t)D(H) = D(H)$ *and* $[U(t), H] = 0$ *on* $D(H)$.
(*d*) *Let* $\psi_0 \in D(H)$. *Then* $U(t)\psi_0$ *uniquely solves the initial value problem*

$$\begin{cases} i\partial_t\psi(t) = H\psi(t) \\ \psi(0) = \psi_0, \end{cases} \tag{1}$$

called the ***Schrödinger equation***.

Hence every self-adjoint operator H generates a strongly continuous one-parameter unitary group $U(t) = e^{-itH}$. A converse is given by ***Stone's theorem***, which states that any weakly continuous one-parameter unitary group gives rise to a self-adjoint operator H such that $U(t) = e^{-itH}$.

Theorem 1.7 (Stone). *Let* $U : \mathbb{R} \to \mathcal{L}(\mathcal{H})$ *be a weakly continuous one-parameter unitary group. Define* $H : D(H) \to \mathcal{H}$ *by*

$$D(H) := \left\{\psi \in \mathcal{H} : \lim_{t\to 0} 1/t(U(t)\psi - \psi) \text{ exists}\right\}$$

and

$$H\psi := \lim_{t\to 0}\frac{i}{t}(U(t)\psi - \psi).$$

Then H *is self-adjoint and* $U(t) = e^{-itH}$.

Wiener and RAGE-Theorem.

Perturbation Theory

Theorem 1.8 (Kato-Rellich). *Let* A *be self-adjoint and* B *symmetric bounded with respect to* A *with* A*-bound less than one. Then* $A + B$ *on* $D(A + B) := D(A)$ *is self-adjoint.*

Next we want to investigate if other properties are preserved by perturbations. Clearly, eigenvalues are not preserved. However, we can remove them from the spectrum.

Corollary 1.1. *Let* A *be self-adjoint and* K *self-adjoint and (relatively) compact. Then* $\sigma_{\text{ess}}(A+K) = \sigma_{\text{ess}}(A)$, *where* $\sigma_{\text{ess}}(A) := \{\lambda \in \sigma(A) : \forall\varepsilon > 0 \operatorname{rank} P^A(\lambda-\varepsilon, \lambda+\varepsilon) = \infty\}$

Proof. Use Weyl characterization of the essential spectrum via ***singular Weyl sequences*** (Weyl sequencenses where additionally $\psi_n \rightharpoonup 0$). □

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Time Evolution of explicit Operators

Examples 1.2. Let us consider some explicit self-adjoint operators H.
(a) (***Free Particles***) $\mathcal{H} := L^2(\mathbb{R}^d, dx)$ and $H := -\Delta$. Then

$$\sigma(H) = \sigma_{\mathrm{ac}}(A) = [0, \infty).$$

(b) (***Harmonic Oscillator***) $\mathcal{H} := L^2(\mathbb{R}^d, dx)$ and $H := -\Delta + \omega^2 x^2$, for some $\omega \in \mathbb{R}$. Then

$$\sigma(H) = \sigma_{\mathrm{pp}}(H) = \omega(2\mathbb{N} + 1).$$

(c) (***One dimensional System***) $\mathcal{H} := L^2(\mathbb{R}^d, dx)$ and $H := -\Delta + V(x)$, where

$$V(x) := \begin{cases} -b & |x| < a, \\ 0 & |x| \geq a. \end{cases}$$

for some $a, b > 0$. Then

$$\sigma_{\mathrm{ess}}(H) = \sigma_{\mathrm{ess}}(-\Delta) = [0, \infty)$$

by Weyl's theorem and we can ask for eigenvalues.
(d) (***Hydrogen Atom***) $\mathcal{H} := L^2(\mathbb{R}^3, dx)$ and $H := -\Delta - \frac{1}{|x|}$ (use the invariance of H under rotations to solve the stationary Schödinger equation). Then

$$\sigma(H) = \{-1/(4n^2) : n \in \mathbb{N}\} \cup [0, \infty).$$

Stationary States of General Schrödinger Operators

Consider $H := -\Delta + V(x)$, for V locally integrable on $\mathbb{R}^n$. Moreover, consider

$$\varepsilon(\psi) := \langle \psi, H\psi \rangle.$$

We are looking for *existence of minimizers of* ε. First of all, *boundedness from below* is required. Then we get a *variational characterization of the smallest eigenvalue of* H. Then *variational characterization of all the negative eigenvalues of* H.

Semiclassical Approximations

Obtaining informations on eigenvalues of a Schrödinger operator by considering the classical system. We consider here only a Dirichlet-boundary value problem for the Laplacian for bounded open $\Omega \subseteq \mathbb{R}^n$.